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Interaction of Scots Pine Defensin with Model Membrane by Coarse-Grained Molecular Dynamics

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Abstract

© 2017, Springer Science+Business Media New York.Plant defensins are a part of the innate immune system of plants that acts against a broad range of pathogens. Many plant defensins, including pine defensins, show strong antifungal activity that is associated with their ability to penetrate into the fungal cell membrane. However, the exact molecular mechanism of their action remains poorly defined. To obtain insight into the mechanism of protein–membrane interaction, we applied a coarse-grained molecular dynamics simulation to study the interaction of pine defensin with two model membranes: the first consisted of zwitterion-neutral POPC molecules and the second was composed of combined anionic POPG and POPC. The simulations show that defensin does not form stable complexes with the neutral membrane but does interact with the combined POPG/POPC membrane. In the latter case, defensin attaches to the membrane surface by interacting with lipid polar heads without deep penetration into the hydrophobic tail zone. Electrostatic interactions are a driving force of the complex formation, which determines the orientation of the protein relative to the bilayer surface. Two favorable orientations of defensin are detected where the defensin molecule orients either perpendicular or parallel to the membrane plane. Being positively charged, pine defensin induces changes in the lipid distribution along the membrane, resulting in the formation of zones with different electrostatic potentials that can cause deformation or distortion of the membrane. Pine defensin is a representative of plant defensins, and hence the results of this study can be applied to other members of the family.

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Keywords

Coarse-grained molecular dynamics, Defensin, Lipid–protein interactions, Membrane

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